Finding k-best MAP Solutions Using LP Relaxations

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Prediction Problems

- Consider the following problem:
  - Observe variables: $\boldsymbol{x}^v$
  - Predict variables: $\boldsymbol{x}^h$

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  - Observe variables: x^v
  - Predict variables: x^h
- Countless applications:
  - Images:
  - Error correcting codes
  - Medical diagnostics
  - Text

Visible	Hidden
Noisy Image	Source Image
Received bits	Code word
Symptoms	Disease
Sentence	Derivation

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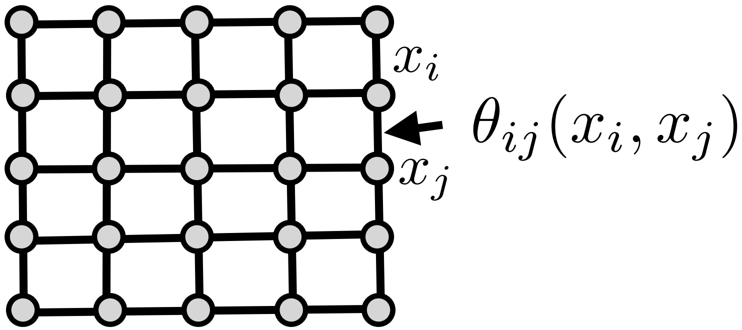
  - This conditional distribution often corresponds to a graphical model
  - Need to know how to find an assignment with maximum probability

The MAP Problem

- Given a graphical model over $x_1, \ldots, x_n$

$$p(\boldsymbol{x}) = \frac{1}{Z} e^{f(\boldsymbol{x})}$$

$$f(\boldsymbol{x}) = \sum_{ij} \theta_{ij}(x_i, x_j)$$



- Find the most likely assignment: $\arg\max_{\boldsymbol{x}} f(\boldsymbol{x})$

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  - Can be solved via message passing

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  - Supervised learning

From 2 to k best

- We can show that given a polynomial algorithm for k=2, the problem can be solved for any k in O(k)
- Focus on k=2
- Our key question: what is the LP formulation of the problem, and its relaxations?

Outline

- LP formulation of the MAP problem
- LP for 2nd best
  - General (intractable) exact formulation
  - Tractable formulation for tree graphs
  - Approximations for non-tree graphs
- Experiments

MAP and LP

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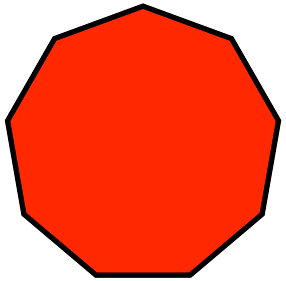

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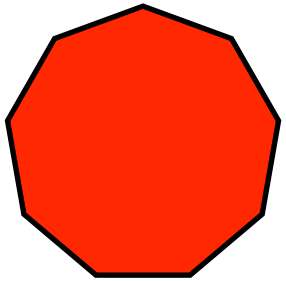

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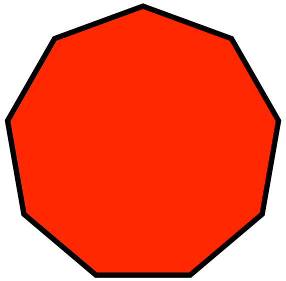

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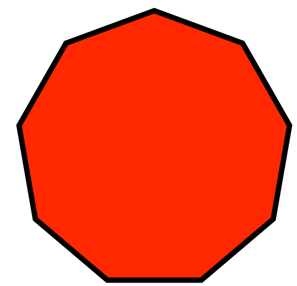

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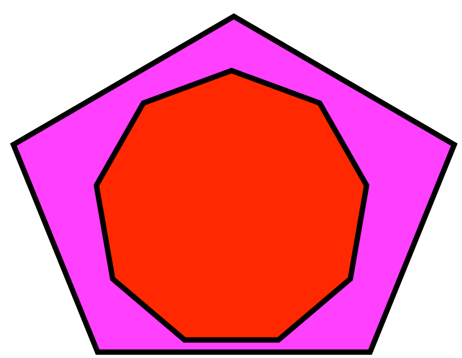

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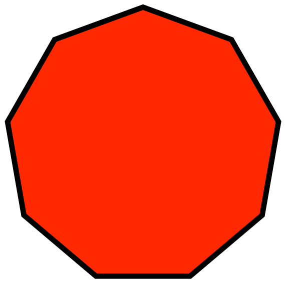

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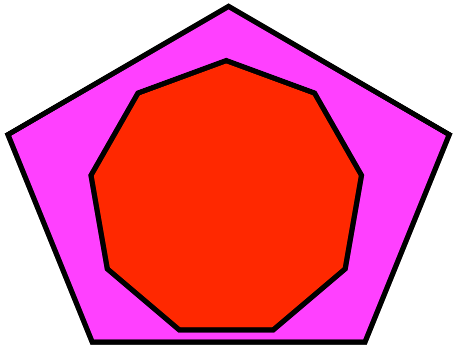

Schlesinger, Deza & Laurent, Boros, Wainwright, Kolmogorov

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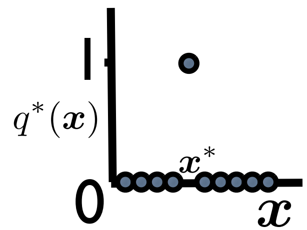

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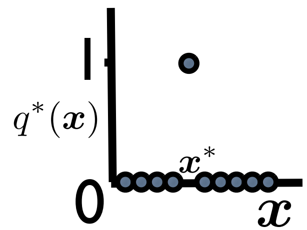

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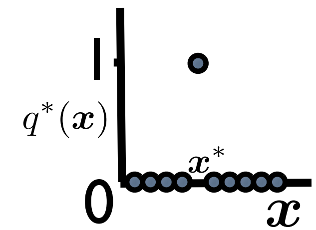

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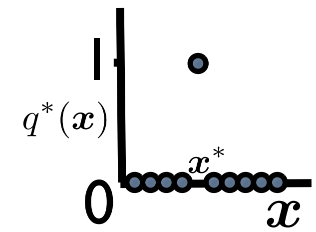

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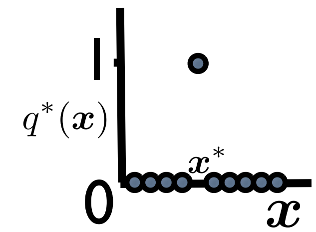

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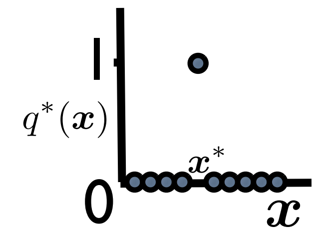

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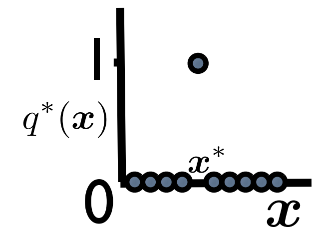

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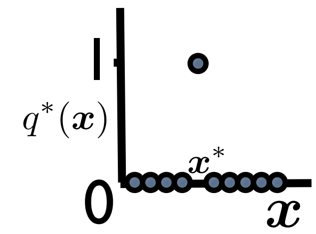

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See: Cut polytope (Deza, Laurent),
Quadric polytope (Boros)

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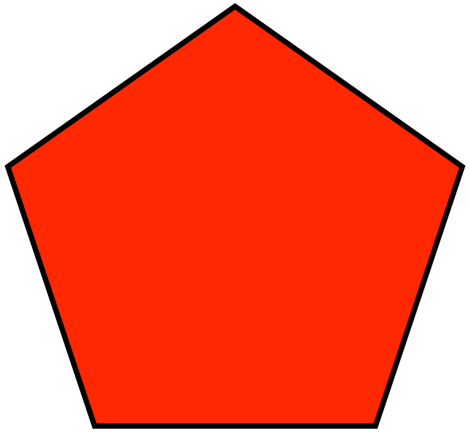

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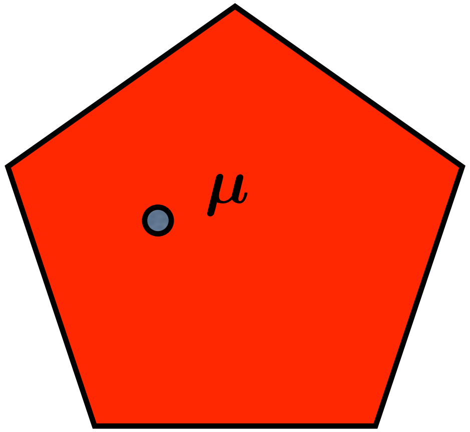

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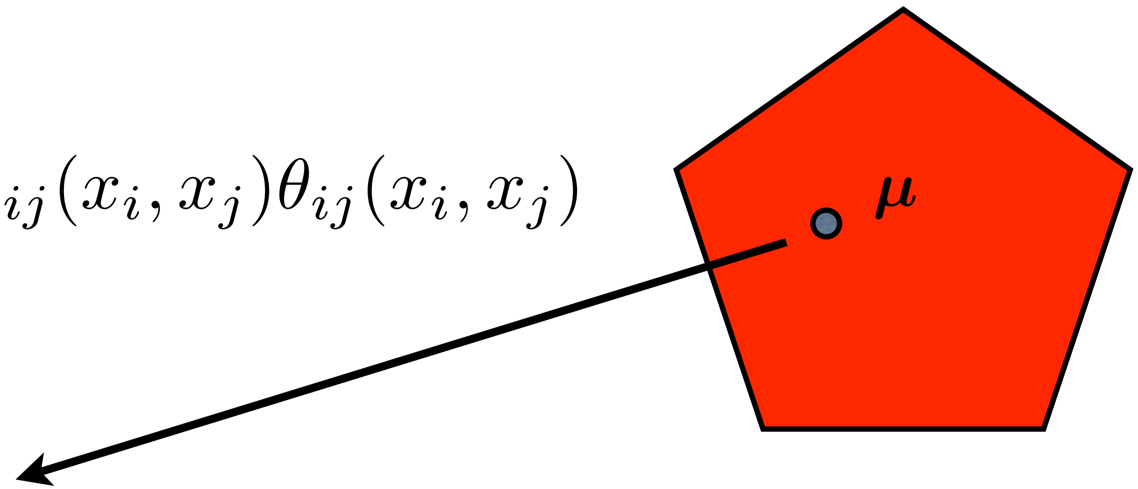

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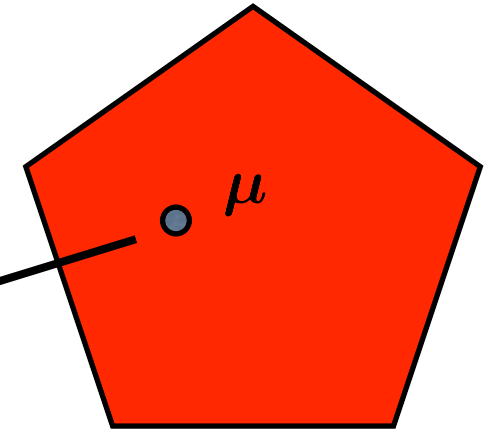

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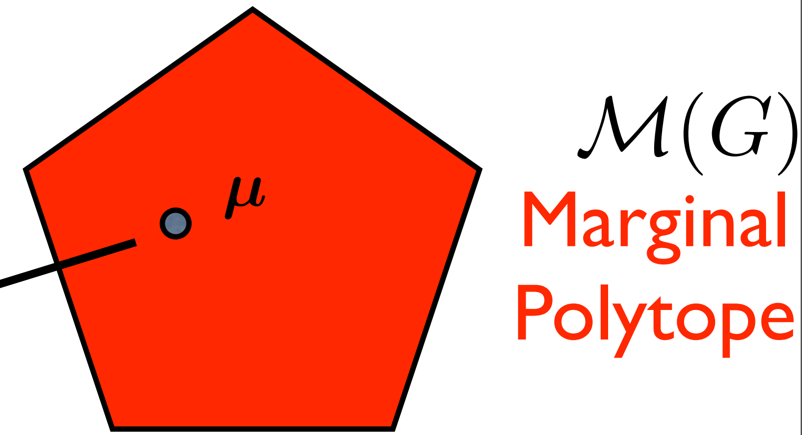

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- The vertices have integral values and correspond to assignments on **x**

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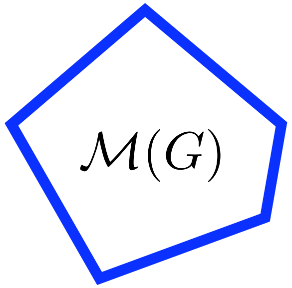

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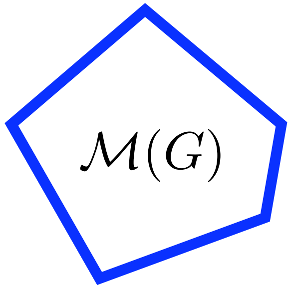

Exact but Hard!

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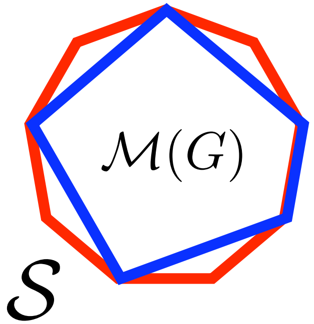

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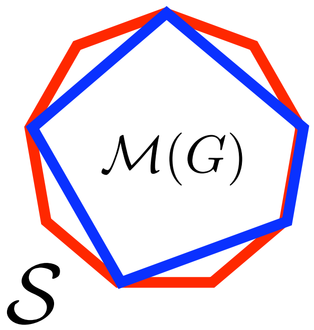

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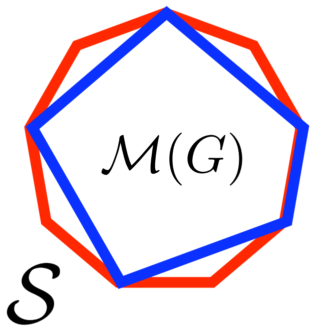

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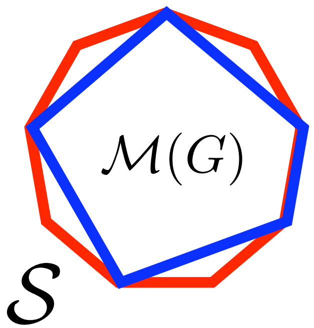

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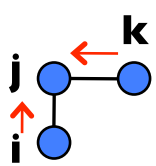

$$\sum_{x_i} \mu_{ij}(x_i, x_j) = \sum_{x_k} \mu_{jk}(x_j, x_k)$$

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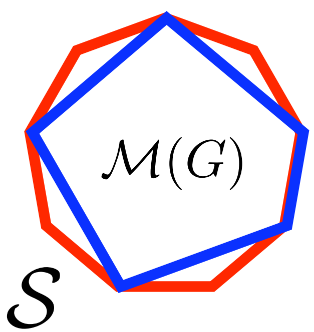
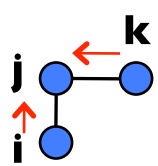
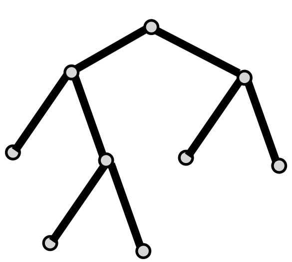


- If optimum is an integral vertex, MAP is solved
- Possible outer bound: Pairwise consistency



$$\sum_{x_i} \mu_{ij}(x_i, x_j) = \sum_{x_k} \mu_{jk}(x_j, x_k)$$

Exact for trees



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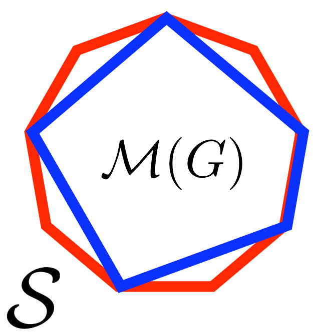

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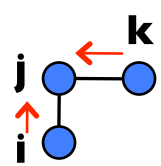

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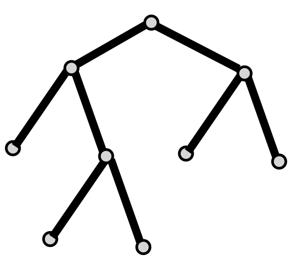

- Efficient message passing schemes for solving the resulting (dual) LP

Outline

- LP formulation of the MAP problem
- LP for 2nd best
  - General (intractable) exact formulation
  - Tractable formulation for tree graphs
  - Approximations for non-tree graphs
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The 2nd best problem and LP

MAP

2nd best

The 2nd best problem and LP

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$$\max_{\boldsymbol{x}} f(\boldsymbol{x})$$

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The 2nd best problem and LP

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The 2nd best problem and LP

<u>MAP</u>

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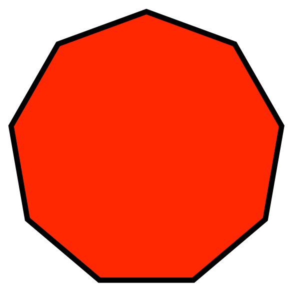

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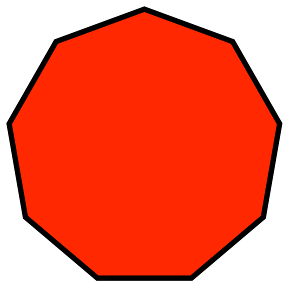

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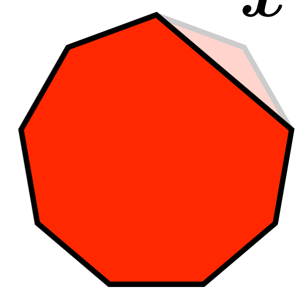

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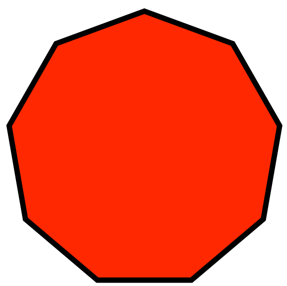

Approximations:

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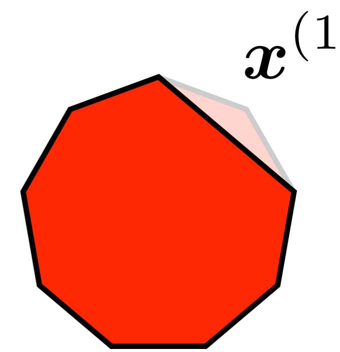

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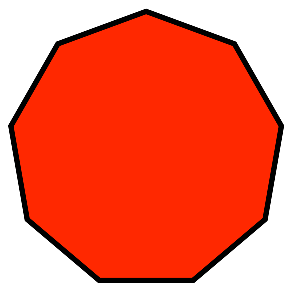

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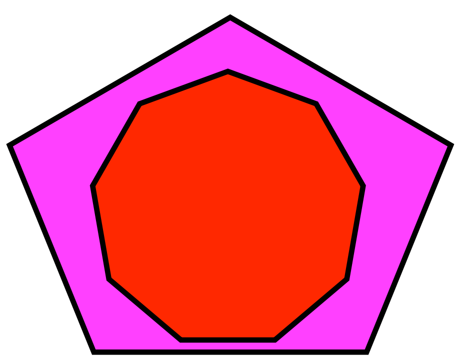

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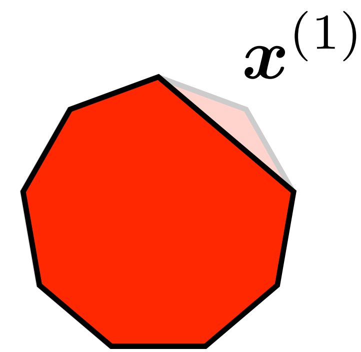

The 2$^{\text{nd}}$ best problem and LP

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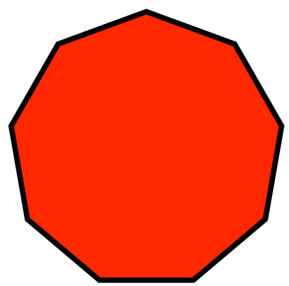

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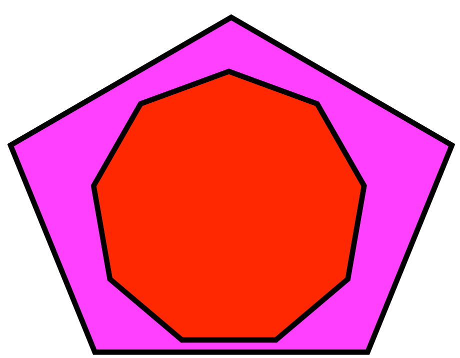

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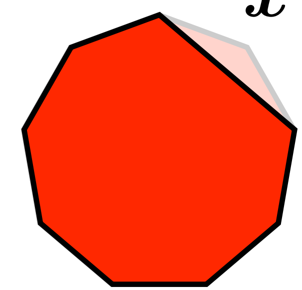

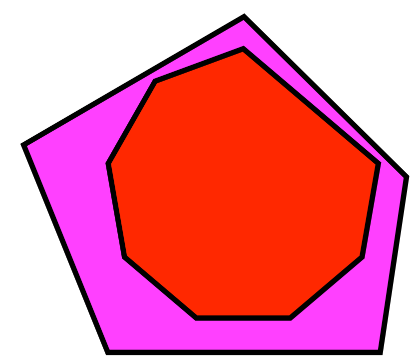

A new marginal polytope

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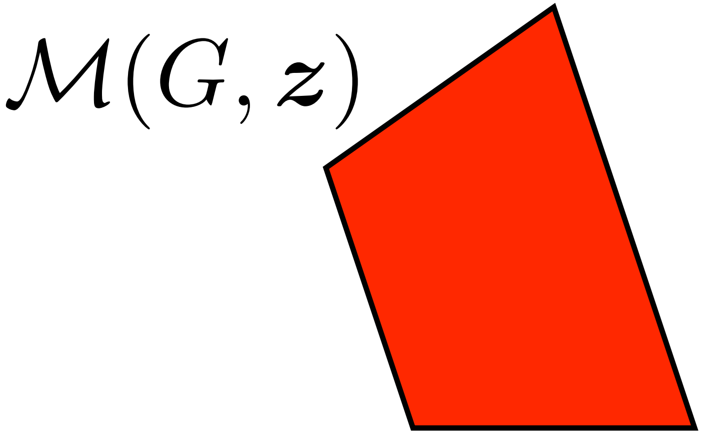

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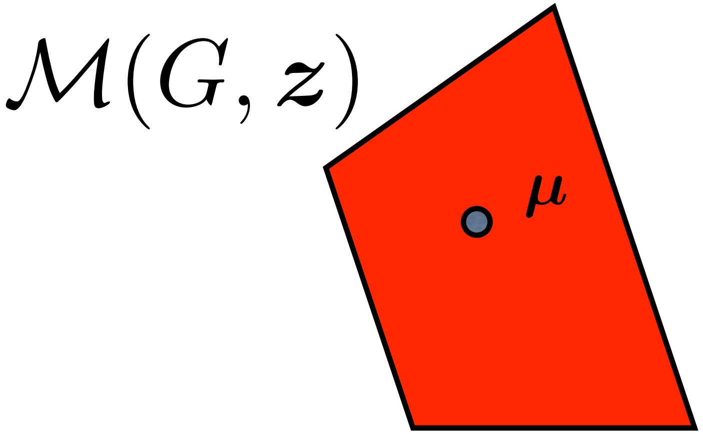

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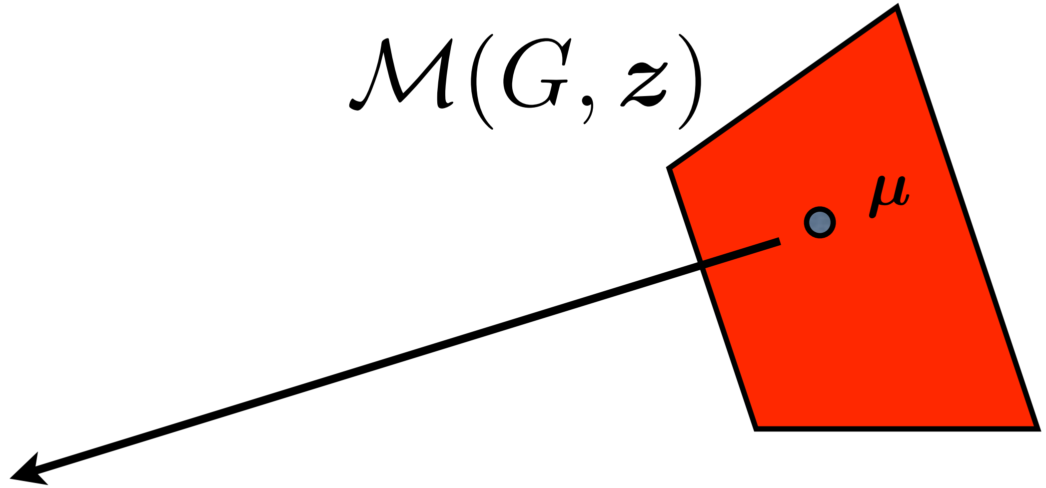

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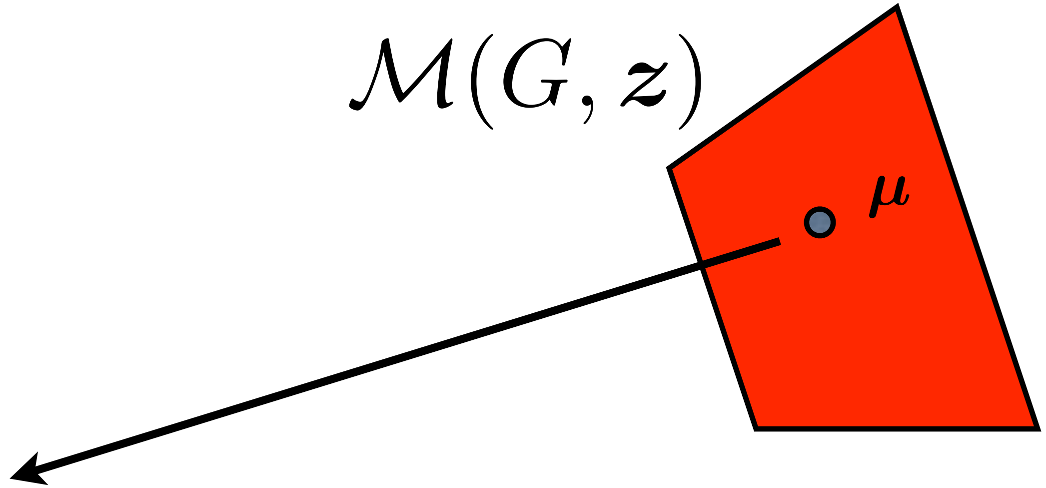

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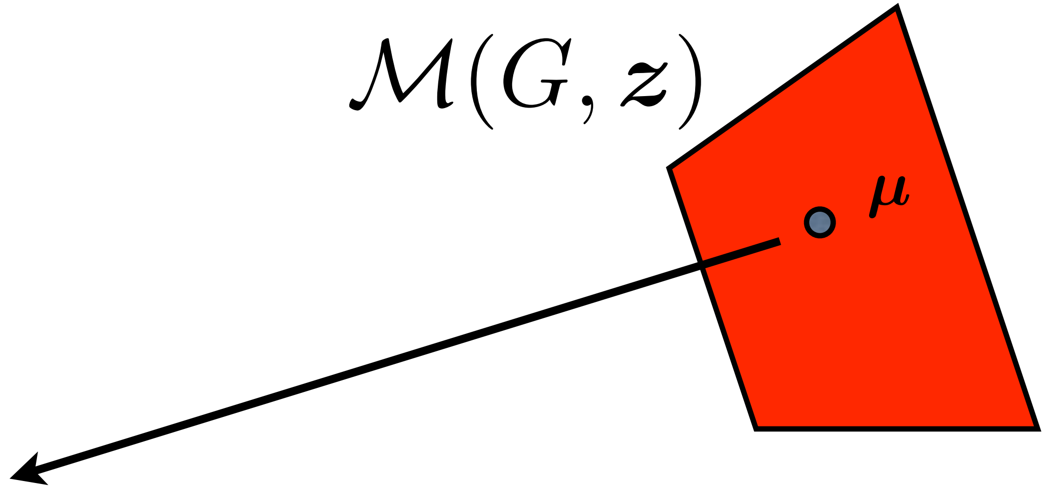

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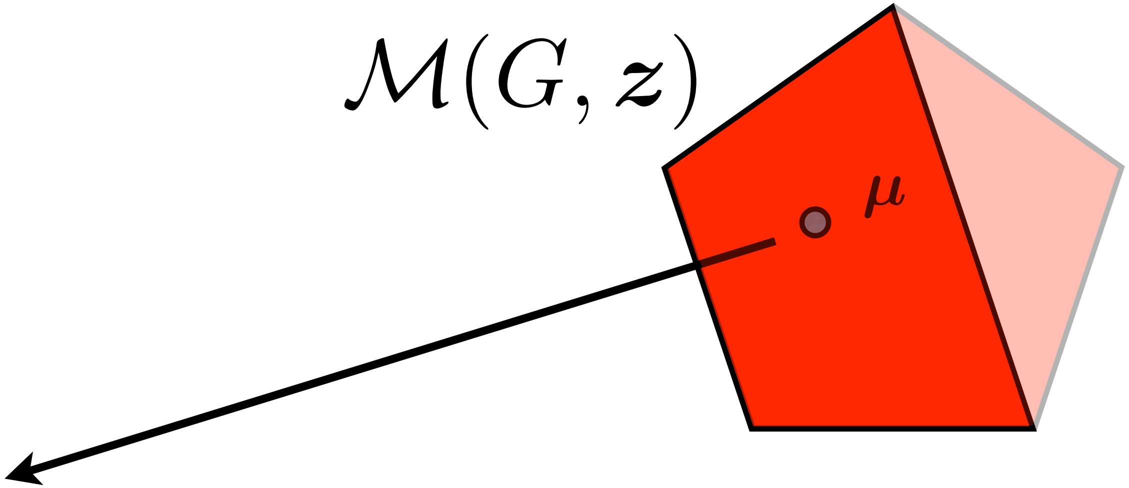

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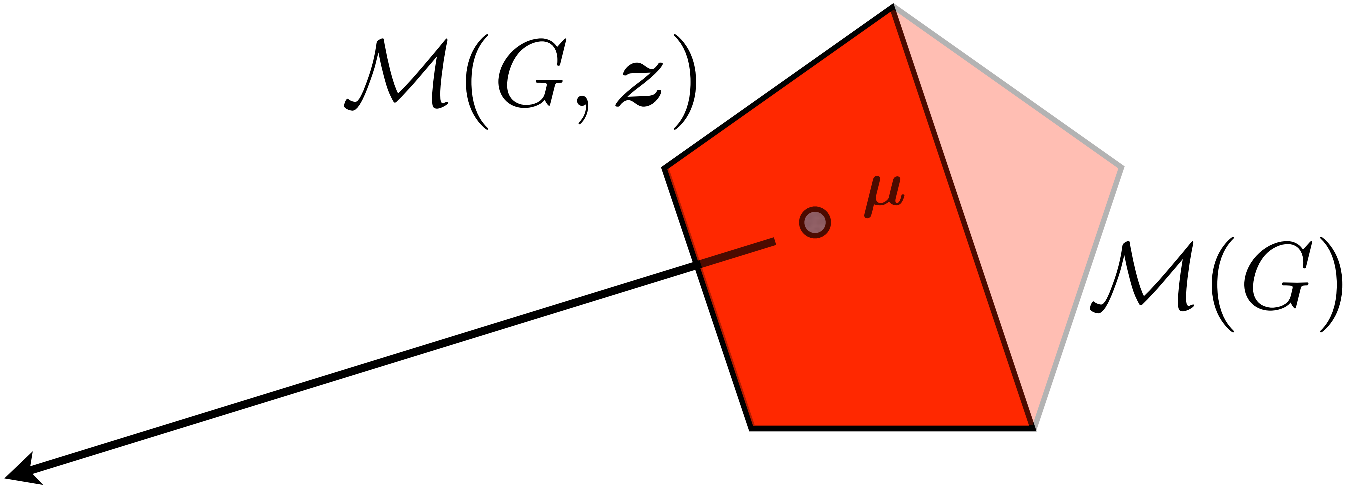

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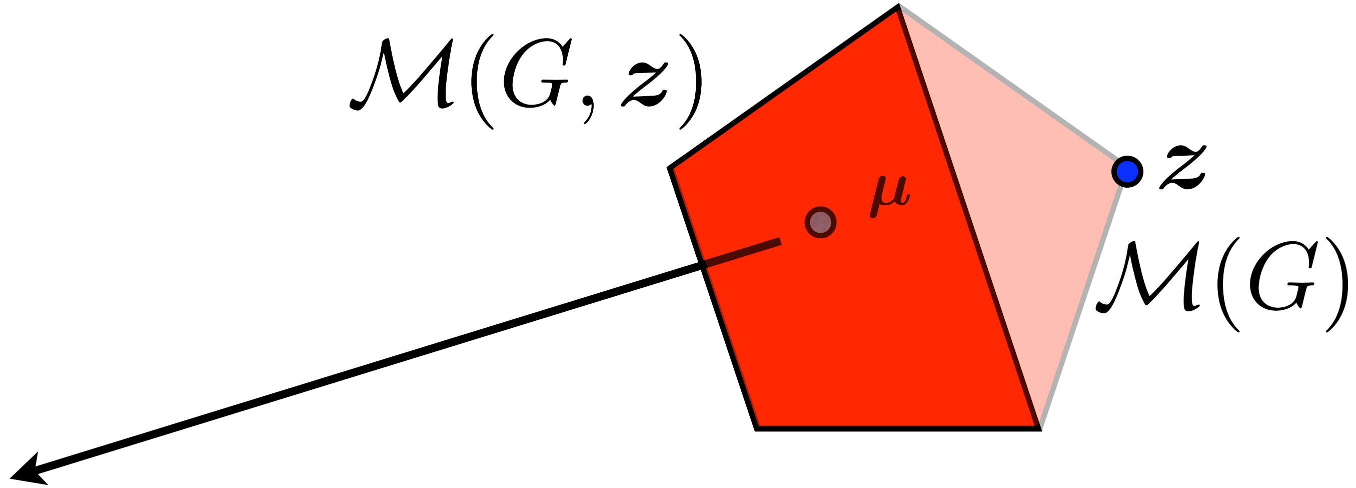

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LP for the 2nd best problem

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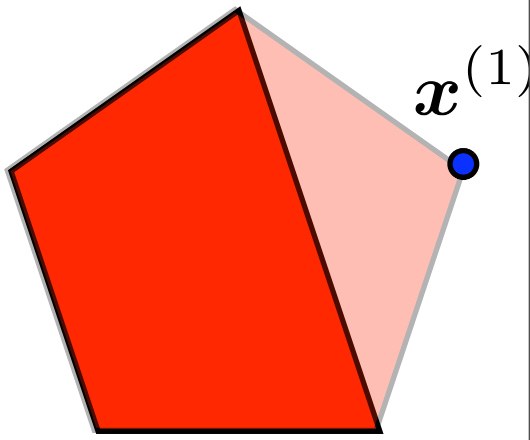
$$\max_{\boldsymbol{x} \neq \boldsymbol{x}^{(1)}} f(\boldsymbol{x}; \boldsymbol{\theta}) = \max_{\boldsymbol{\mu} \in \mathcal{M}(G, \boldsymbol{x}^{(1)})} \boldsymbol{\mu} \cdot \boldsymbol{\theta}$$



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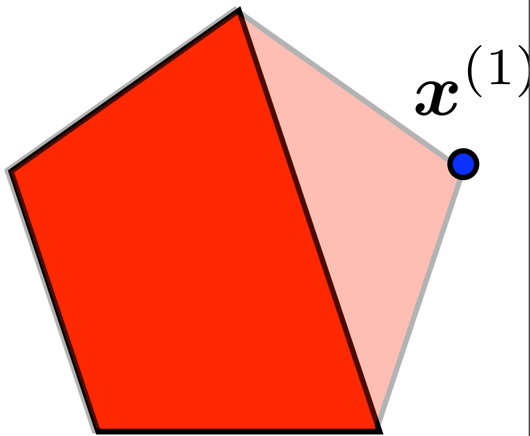

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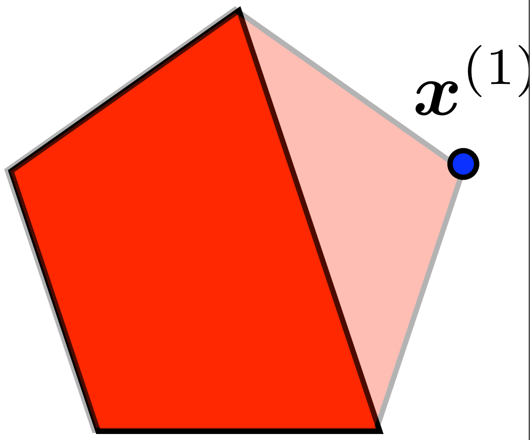

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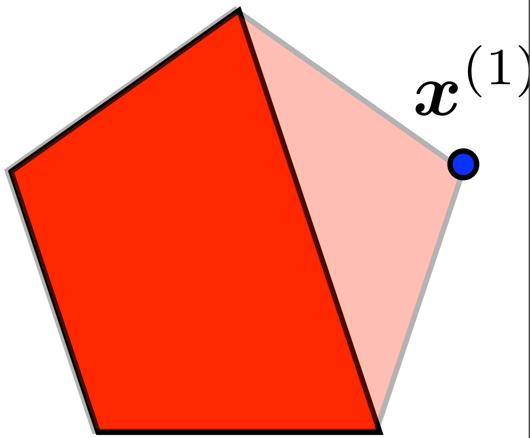

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Outline

- LP formulation of the MAP problem
- LP for 2^{nd} best
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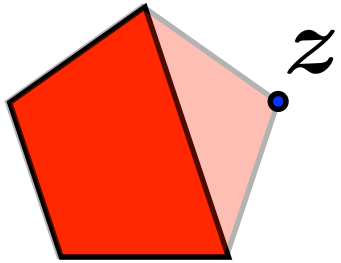
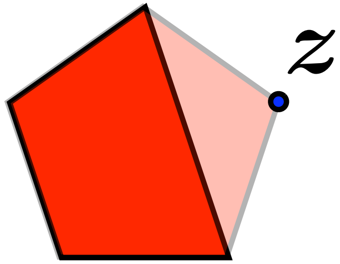
Adding inequalities to $\mathcal{M}(G)$

z



Adding inequalities to $\mathcal{M}(G)$

- Any valid inequality must separate z from the other vertices



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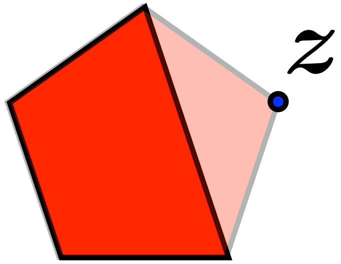

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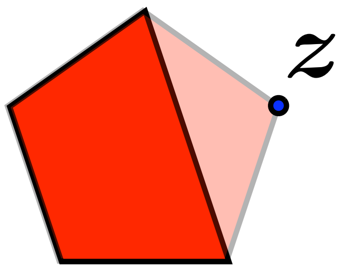

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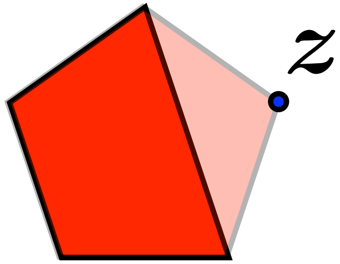

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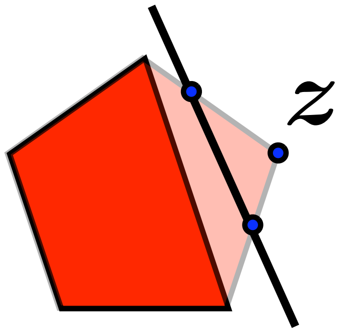

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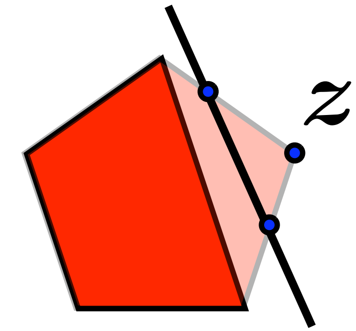

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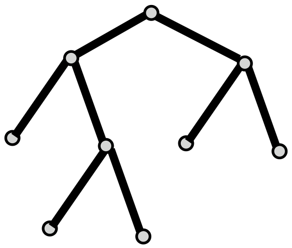
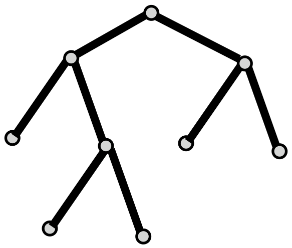
- Only an outer bound on $\mathcal{M}(G, z)$

The tree case



The tree case

- Focus on the case where G is a tree



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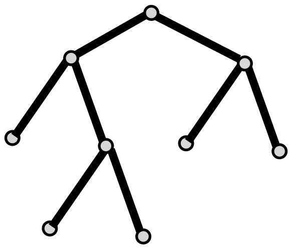

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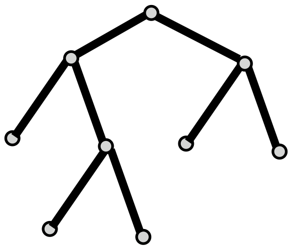

$$\boxed{I(\boldsymbol{\mu}, \boldsymbol{z}) = \sum_i (1 - d_i)\mu_i(z_i) + \sum_{ij \in G} \mu_{ij}(z_i, z_j)}$$

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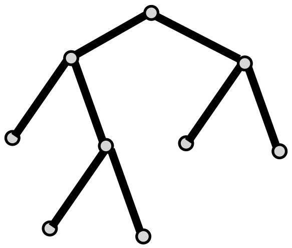

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Bethe: $H(\boldsymbol{\mu}) = \sum_i (1 - d_i) H_i(X_i) + \sum_{ij \in G} H(X_i, X_j)$

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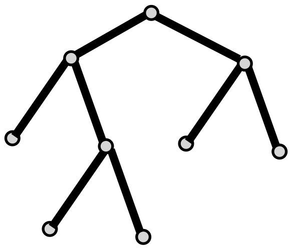

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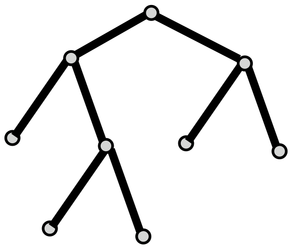

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- <u>Theorem:</u>

$$\mathcal{M}(G, \boldsymbol{z}) = \{\boldsymbol{\mu} \mid \quad \boldsymbol{\mu} \in \mathcal{M}(G), \quad I(\boldsymbol{\mu}, \boldsymbol{z}) \leq 0 \ \}$$

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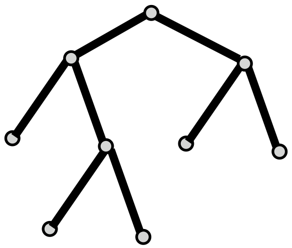

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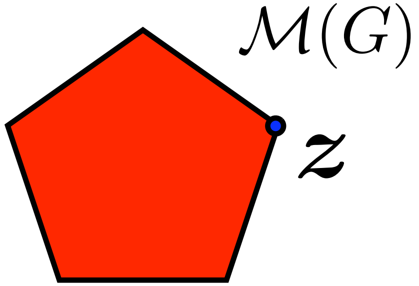
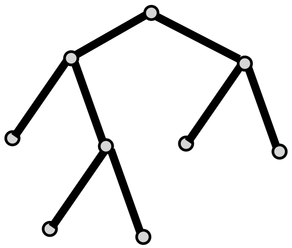


The tree case

- Focus on the case where G is a tree



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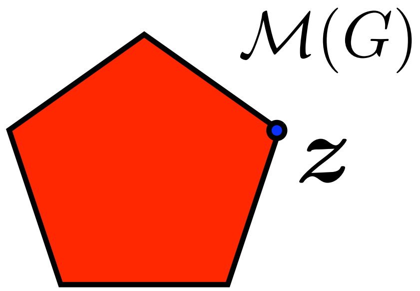

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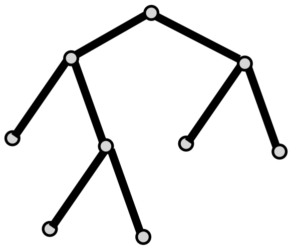

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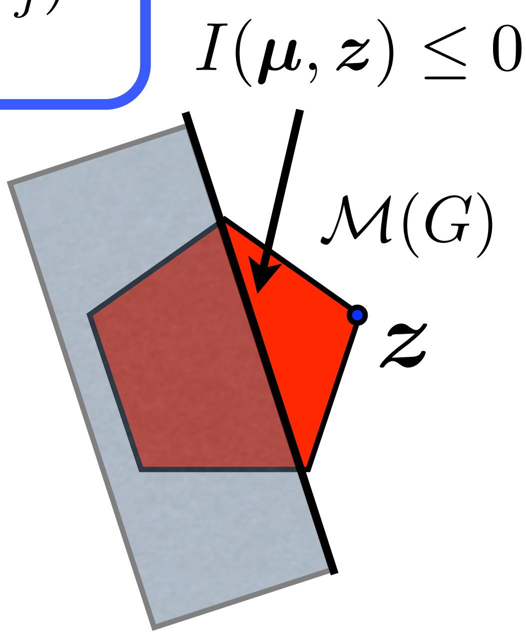

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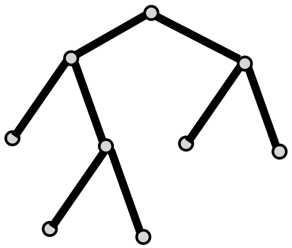

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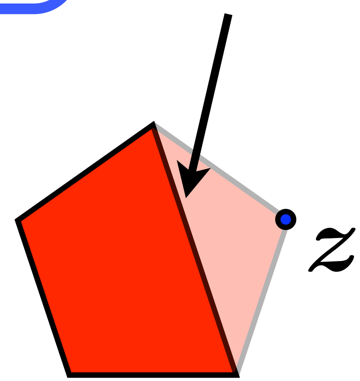

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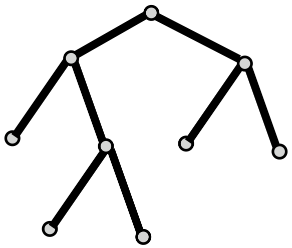

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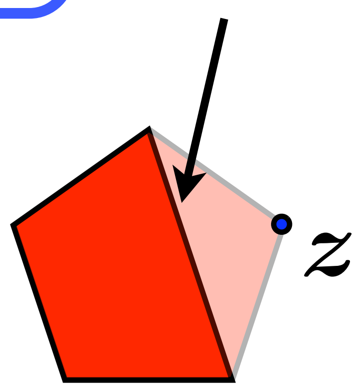

Proof...

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Can construct p(x)

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$$F(\boldsymbol{\mu}) = \left\{ \begin{array}{ll} \min & p(\boldsymbol{z}) \\ \mathrm{s.}t. & p_{ij}(x_i, x_j) = \mu_{ij}(x_i, x_j) \\ & p_i(x_i) = \mu_i(x_i) \\ & p(\boldsymbol{x}) \geq 0 \end{array} \right.$$

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- In fact we can show that for trees:

$$\boldsymbol{\mu} \in \mathcal{M}(G) \implies F(\boldsymbol{\mu}) = \max\{0, I(\boldsymbol{\mu}, \boldsymbol{z})\}$$

Proof - key ideas

$$F(\boldsymbol{\mu}) = \begin{cases} \min & p(\boldsymbol{z}) \\ \text{s.}t. & p_{ij}(x_i, x_j) = \mu_{ij}(x_i, x_j) \\ & p_i(x_i) = \mu_i(x_i) \\ & p(\boldsymbol{x}) \geq 0 \end{cases}$$

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Dual:

$$\begin{array}{ll} \max & \boldsymbol{\lambda} \cdot \boldsymbol{\mu} \\ \text{s.t.} & \sum_{ij} \lambda_{ij}(x_i, x_j) + \sum_i \lambda_i(x_i) \leq 0 \quad \forall \boldsymbol{x} \neq \boldsymbol{z} \\ & \sum_{ij} \lambda_{ij}(\boldsymbol{z}_i, \boldsymbol{z}_j) + \sum_i \lambda_i(\boldsymbol{z}_i) = 1 \end{array}$$

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- We show that the value of the above is $I(\boldsymbol{\mu}, \boldsymbol{z})$

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Proof - Max marginals

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- Rewrite: $\lambda(\boldsymbol{x}) = \sum_i (1 - d_i)\bar{\lambda}(x_i) + \sum_{ij \in T} \bar{\lambda}_{ij}(x_i, x_j)$

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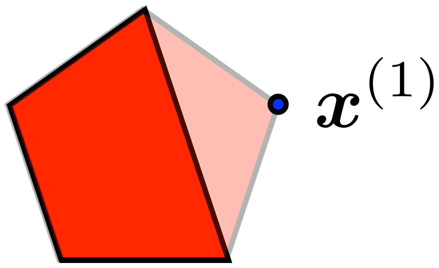
- Rewrite: $\lambda(\boldsymbol{x}) = \sum_i (1 - d_i)\bar{\lambda}(x_i) + \sum_{ij \in T} \bar{\lambda}_{ij}(x_i, x_j)$
- Result follows after some algebra

Tree Graph - Summary

$$\mathcal{M}(G, \boldsymbol{x}^{(1)}) = \{ \boldsymbol{\mu} \mid \quad \boldsymbol{\mu} \in \mathcal{M}(G), \quad I(\boldsymbol{\mu}, \boldsymbol{x}^{(1)}) \leq 0 \ \}$$



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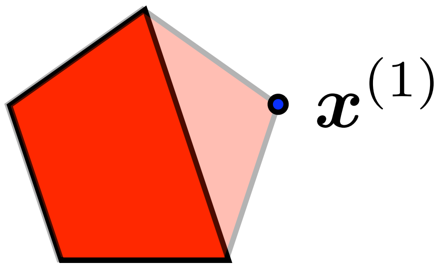
- The LP for 2nd best differs from the marginal polytope by one linear inequality constraint



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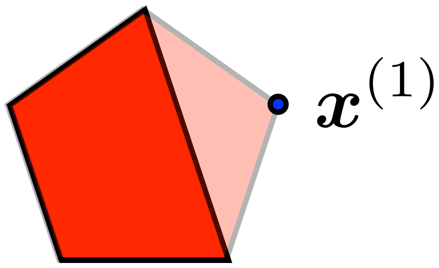

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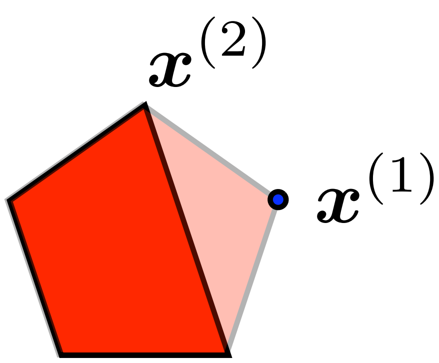

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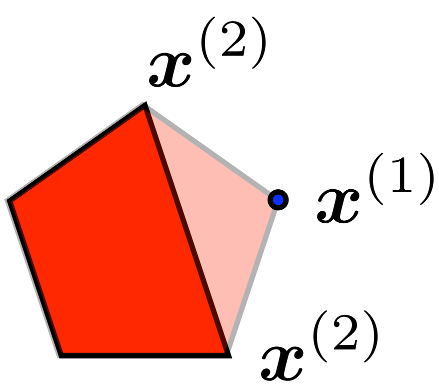

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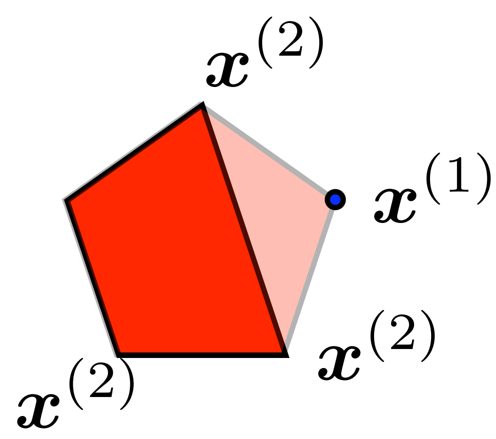

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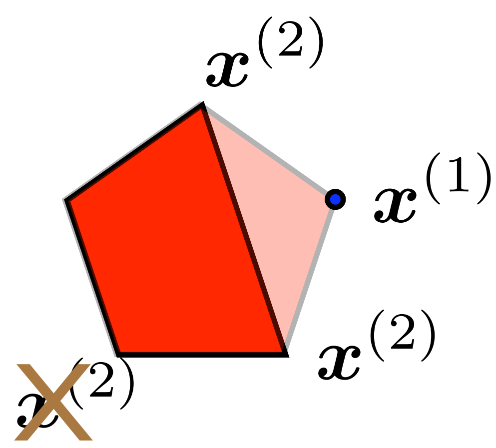

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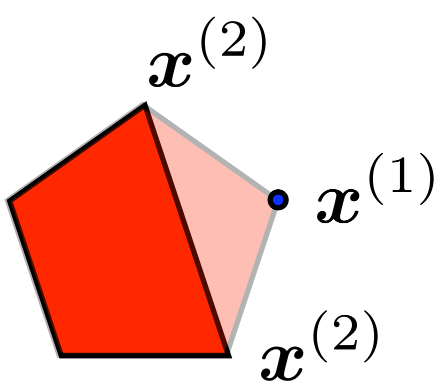
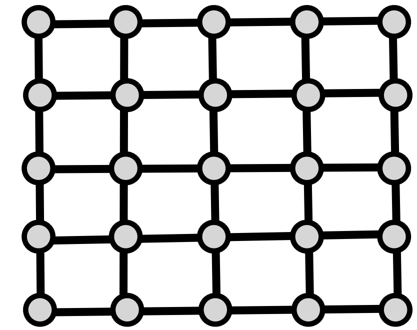


Non tree graphs



- Any graph can be converted into a junction tree
- We can apply our tree result there
- For a junction tree with cliques C and separators S, the inequality is:

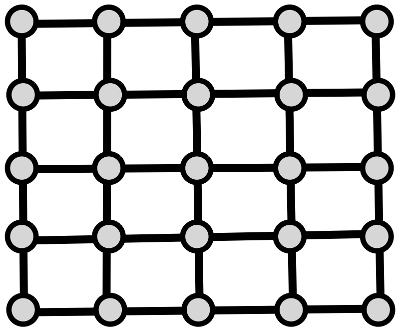
$$\sum_{S \in \mathcal{S}} (1 - d_S)\mu_S(z_S) + \sum_{C \in \mathcal{C}} \mu_C(z_C) \leq 0$$

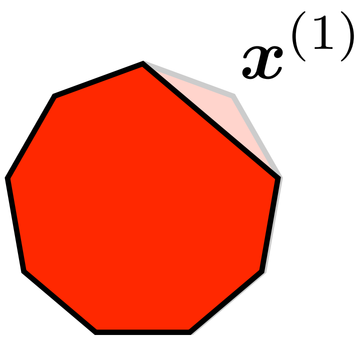
- Specifying the marginal polytope requires a number of variables exponential in the tree width. Not practical.

Outline

- LP formulation of the MAP problem
- LP for 2^{nd} best
  - General (intractable) exact formulation
  - Tractable formulation for tree graphs
  - Approximations for non-tree graphs
- Experiments

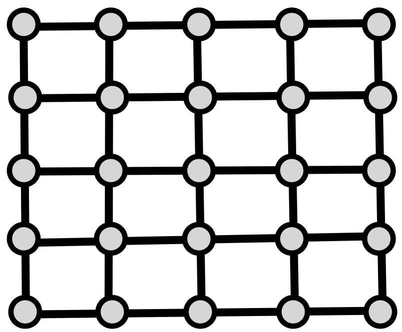
Non trees - Approximations

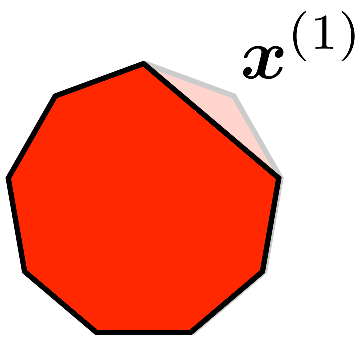


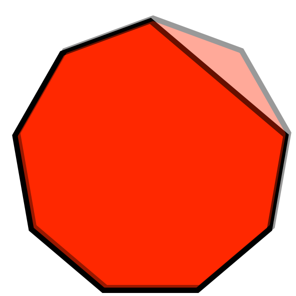


True $\mathcal{M}(G, \boldsymbol{x}^{(1)})$

Non trees - Approximations







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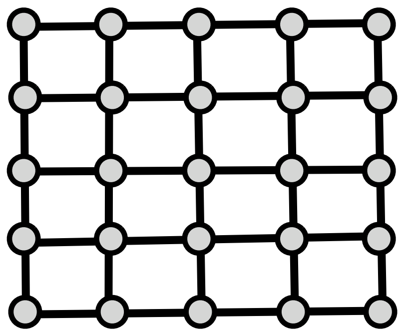

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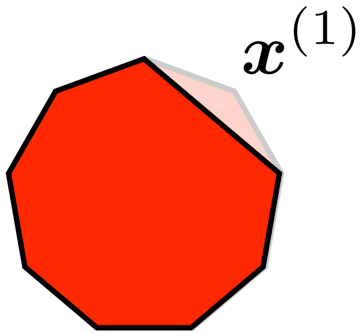

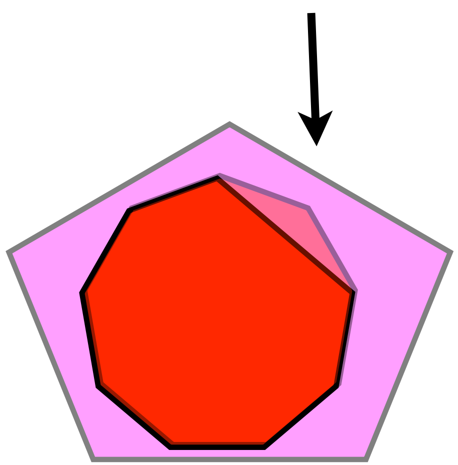

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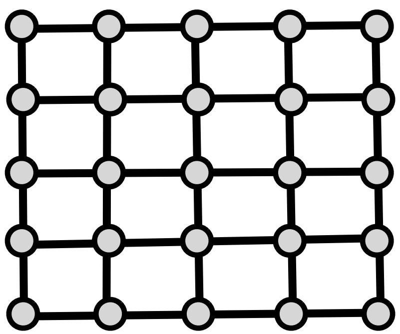

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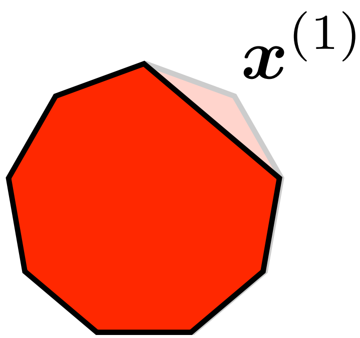

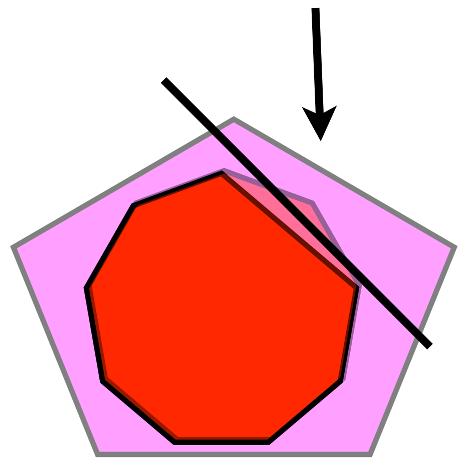

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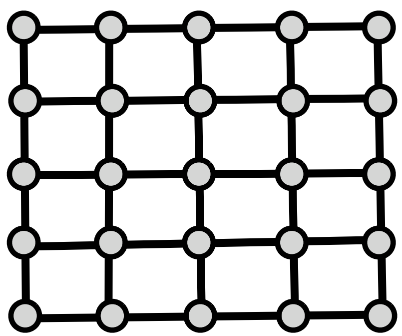

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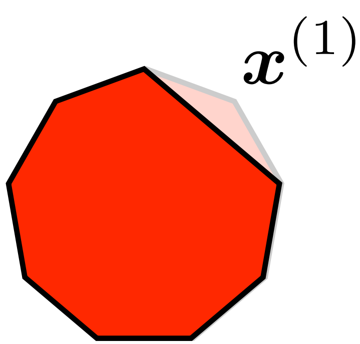

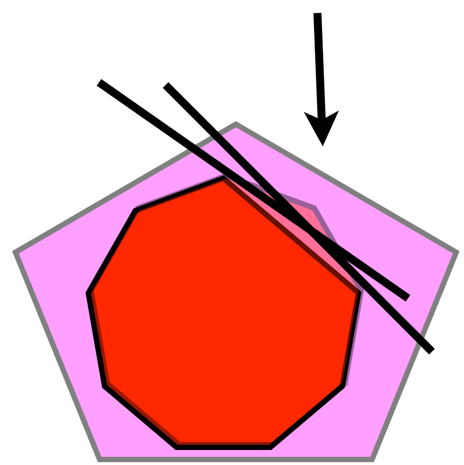

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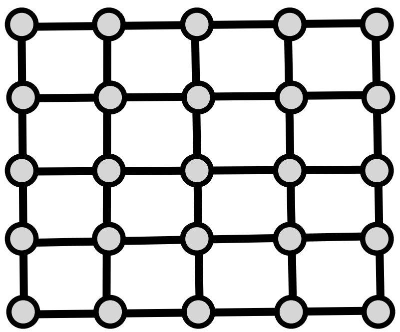

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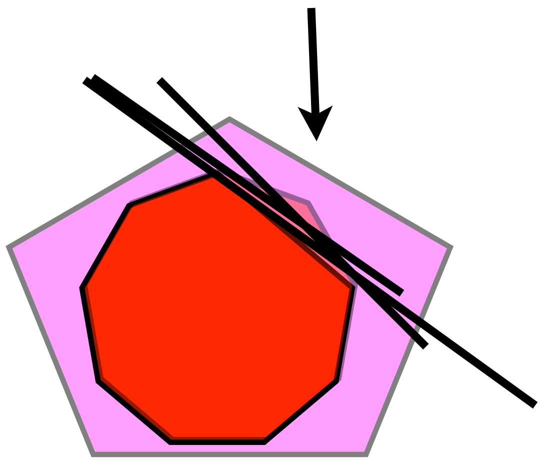

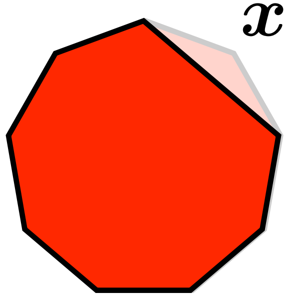

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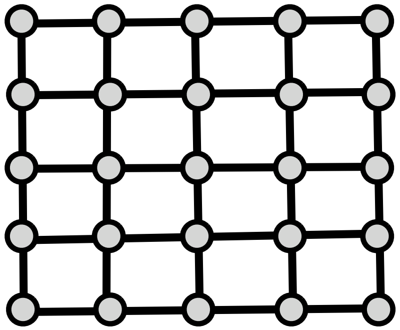
Spanning tree inequalities

- Give a spanning subtree T of G define

$$I^T(\boldsymbol{\mu}, \boldsymbol{z}) = \sum_i (1 - d_i)\mu_i(z_i) + \sum_{ij \in T} \mu_{ij}(z_i, z_j)$$

- And the constraint: $I^T(\boldsymbol{\mu}, \boldsymbol{z}) \leq 0$



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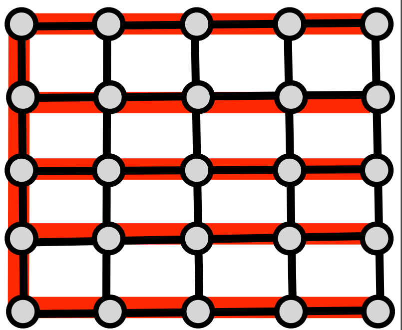

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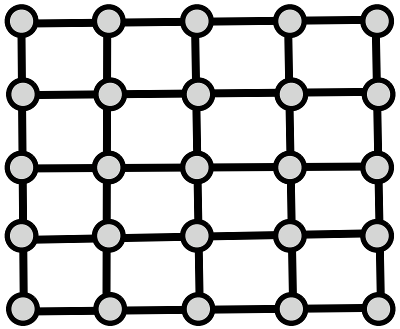

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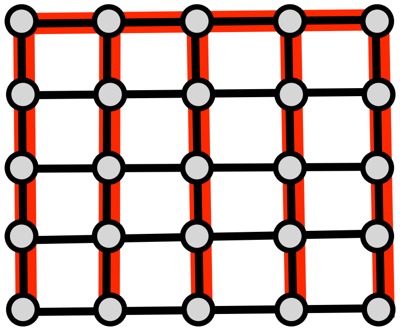

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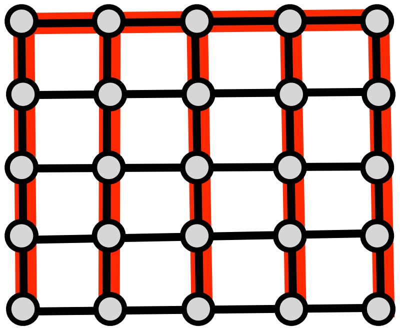

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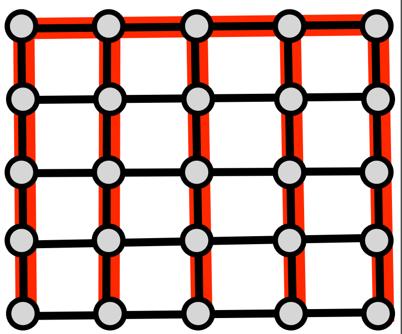

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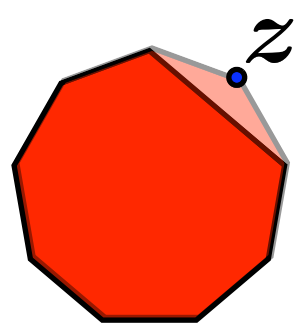

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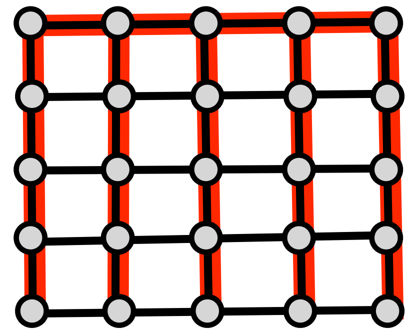

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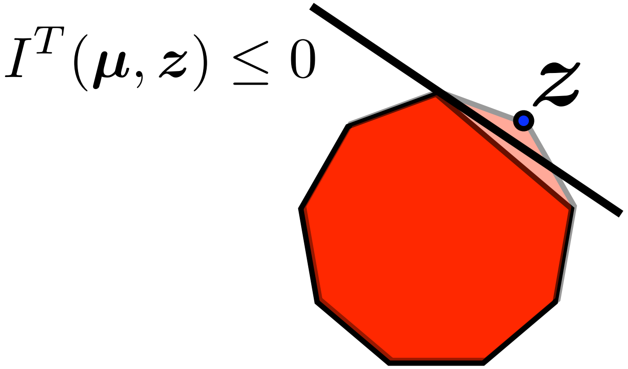

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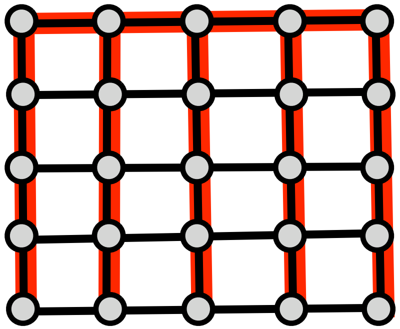

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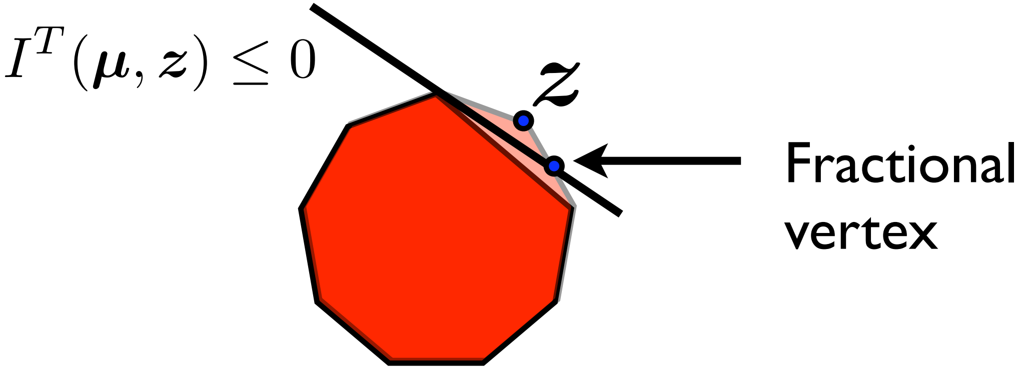

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  - If solution is fractional, find a violated tree inequality (if exists) and add it

Cutting Plane Algorithm

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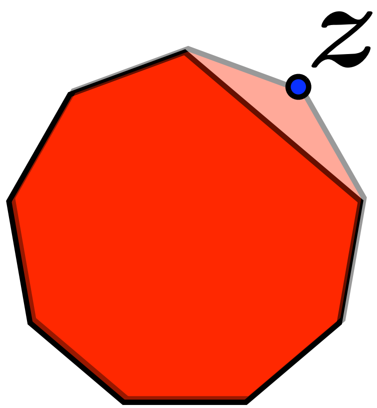

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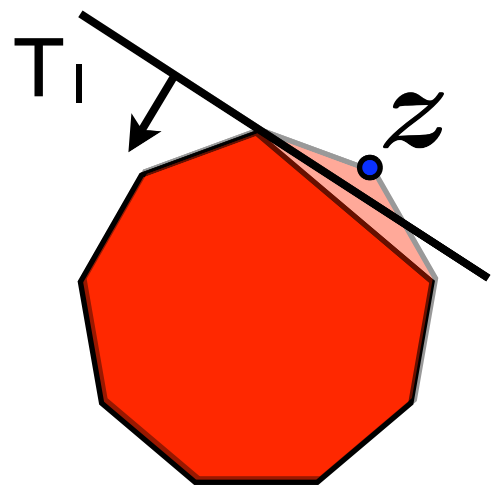

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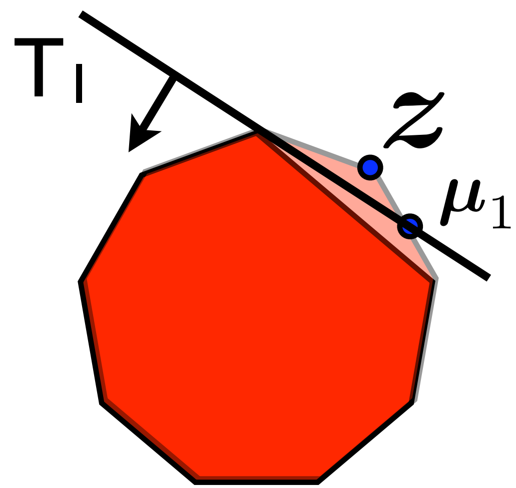

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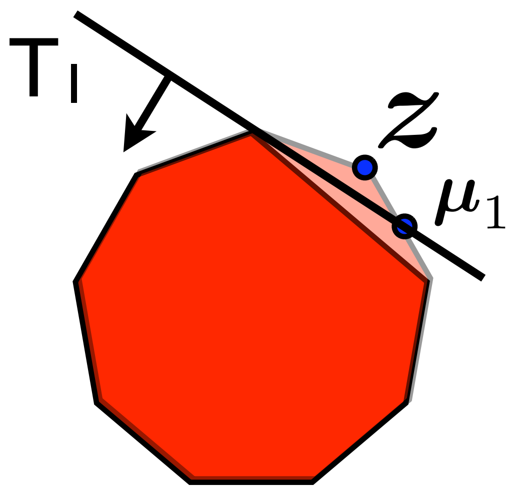

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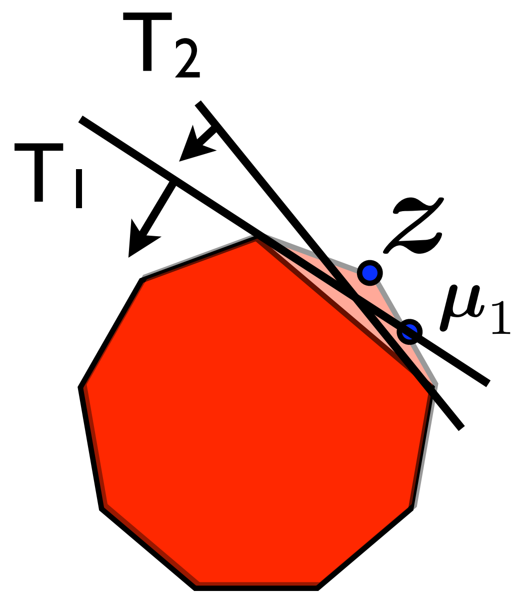

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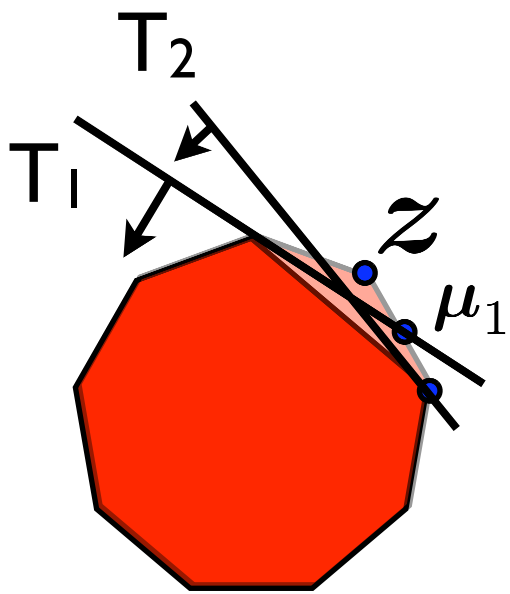

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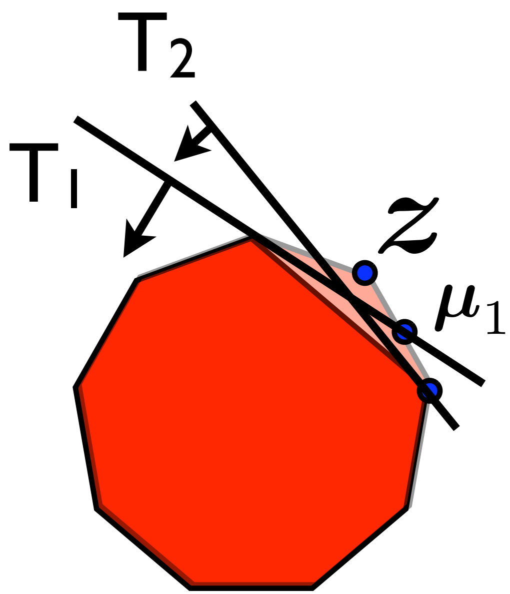

Is there a tree inequality that μ_1 violates?

- How do we find a violated tree inequality?
- Note: Even all spanning tree inequalities might not suffice

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- Decomposes into edge scores. Maximizing tree can be found using a maximum-weight-spanning-tree algorithm (e.g., Wainwright 02)

Experiments

- Alternative algorithms for approximate 2nd best:
  - Using approximate marginals from max-product (BMMF; Yanover and Weiss 04)
  - Lawler/Nillson (72,80) - Partition assignments $\boldsymbol{x} \neq \boldsymbol{x}^{(1)}$:

$$
\begin{array}{l|l|l|l|l|}
x_1 \neq x_1^{(1)} & x_2 = * & x_3 = * & \ldots & x_n = * \\
x_1 = x_1^{(1)} & x_2 \neq x_2^{(1)} & x_3 = * & \ldots & x_n = * \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
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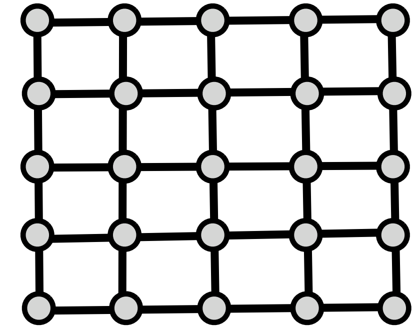
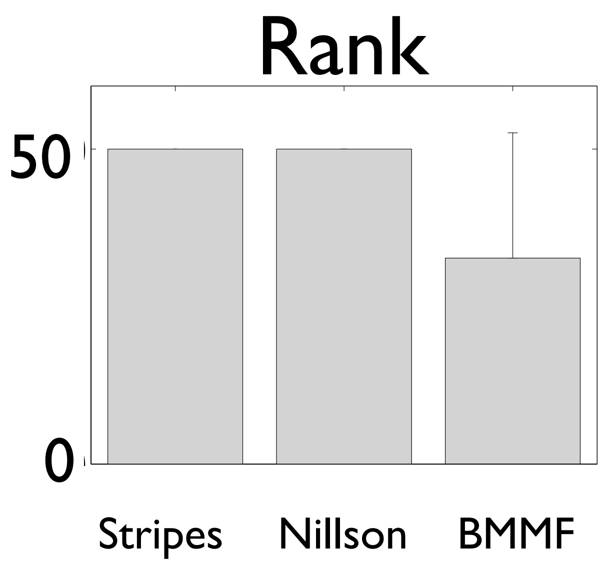
\end{array}
$$

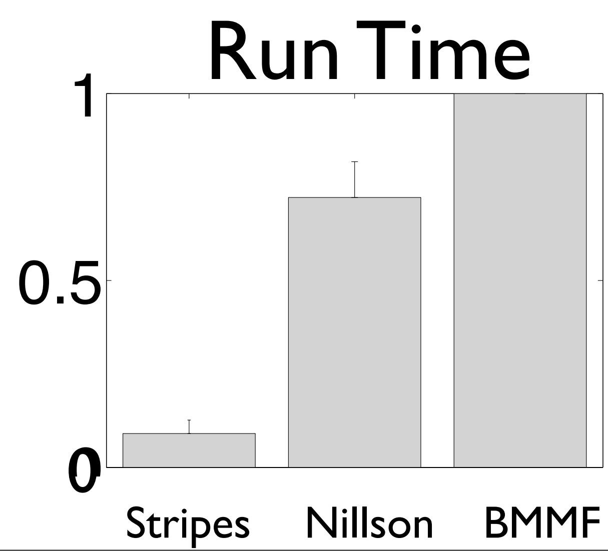
  - Maximize over each part approximately. Cost O(n)
- Our algorithm: STRIPES

Attractive Grids



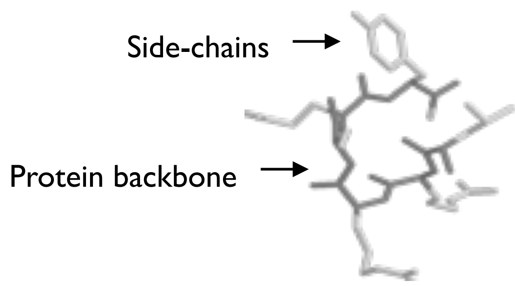
- Ising models with ferromagnetic interaction
- The local-polytope guaranteed to yield exact first best (but not equal to the marginal polytope)
- Goal: Find 50 best. Stripes and Nillson find all of them exactly. Up to 19 spanning trees added



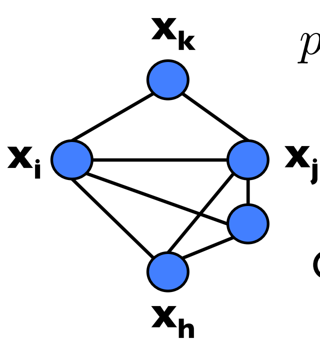


Protein Side Chain Prediction

- Given protein's 3D shape (backbone), choose most probable side chain configuration



(MRFs from Yanover, Meltzer, Weiss '06)

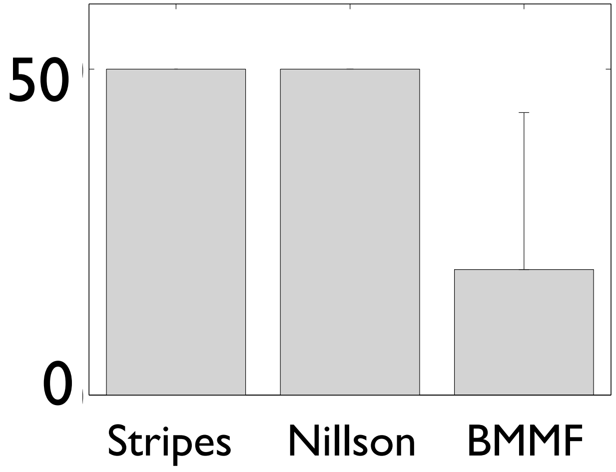


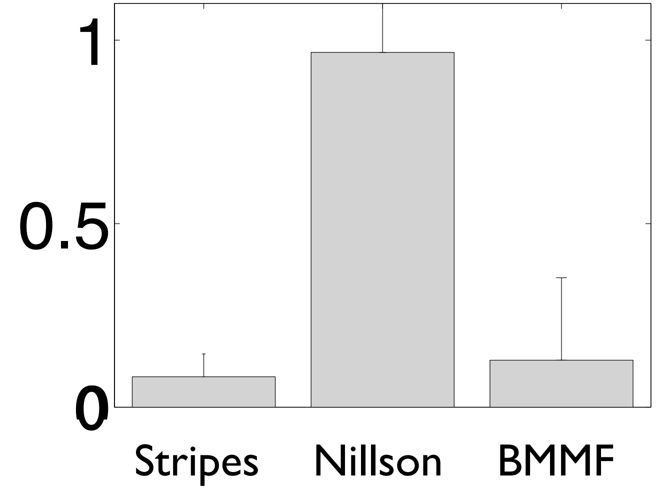
$$p(\boldsymbol{x}) \propto e^{\sum_{ij \in E} \theta_{ij}(x_i, x_j)}$$

- Can be cast as a MAP problem
- Important to obtain multiple possible solutions

Protein Side Chain Prediction

- Stripes found the exact solutions for all problems studied
- In some cases, we used a tighter approximation of the marginal polytope (Sontag et al, UAI 08)





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Summary

- The 2nd best can be posed as a linear program
- For trees differs from 1st best by one constraint only
- For non-trees, approximation can be devised by adding inequalities for all spanning trees
- Empirically effective